Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.09e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.50e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

Image not found
1,5-Naphthalenediamine
Measured: 2.40e-03
Predicted: 6.55e-03

Image not found
1,10-Phenanthroline
Measured: 1.49e-02
Predicted: 5.60e-03

Image not found
1,8-Naphthalenediamine
Measured: 5.37e-03
Predicted: 5.83e-03

Image not found
Etryptamine
Measured: 2.71e-03
Predicted: 5.31e-02

Image not found
4-Aminoacridine
Measured: 6.00e-05
Predicted: 1.96e-02